# Cyclus Fuel Cycle Simulation Capabilities with the Cyder Disposal System Model

## Global 2013

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October 3, 2013

# Outline

1. Motivation
   - Future Fuel Cycle Options
   - Geologic Disposal Concept Options
   - Fuel Cycle Simulator Capabilities
2. Modeling Capabilities
   - Cyder Overview
   - Radionuclide Transport in Cyder
   - Thermal Transport in Cyder
3. Conclusion

# Future Fuel Cycle Options

**Domestic Fuel Cycle Options**

| Title | Description | Challenges |
|---|---|---|
| Open | Once Through<br>Current US PWR Fleet<br>No Separations<br>No Recycling<br>Higher Burnups | High Temperatures, Volumes |
| Modified Open | Partial Recycling<br>Next Gen. PWR Fleet<br>Limited Separations<br>Limited Transmutation<br>Advanced Fuel Forms<br>HLW treatment | Both high volumes and variable spent fuel streams |
| Closed | Full Recycling<br>Full Separations<br>Full Recycling<br>VHTGR, SFRs,<br>other transmutation<br>HLW treatment | Variable spent fuel streams |

Table 1 : Domestic Fuel Cycle Options

# Disposal Geology Options Considered

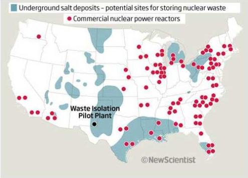


Figure 1 : U.S. Salt Deposits, ref. [20].

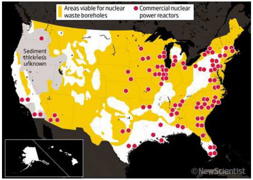


Figure 3 : U.S. Crystalline Basement, ref. [20].

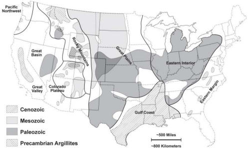


Figure 2 : U.S. Clay Deposits, ref. [6].

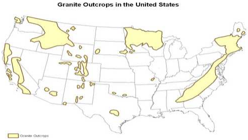
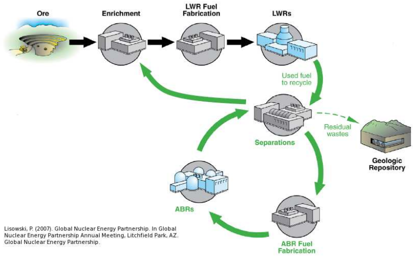


Figure 4 : U.S. Granite Beds, ref. [4].

# Cyclus Top Level Fuel Cycle Simulator



Lisowski, P. (2007). Global Nuclear Energy Partnership. In Global Nuclear Energy Partnership Annual Meeting, Litchfield Park, AZ. Global Nuclear Energy Partnership.

Figure 5 : Top level simulators are intended to model the collective behavior of various fuel cycle decisions and strategies [19].

Figure 6 : cyclus.github.com [12].

# Need For an Integrated Repository Model

**Repository Capabilities within Systems Analysis Tools**

| Tool | Institution | Fuel Disposition | Radionuclide Transport | Heat Transport |
|---|---|---|---|---|
| NUWASTE[1] | NWTRB | yes | no | no |
| VISION [26] | INL | yes | no | YMR only |
| DANESS [24] | ANL | no | no | no |
| COSI [2] | CEA | yes | no | yes |
| NFCSim [21] | LANL | no | no | no |
| CAFCA [9] | MIT | no | no | no |
| ORION [9] | BNL | no | no | no |
| TSM [23] | OCRWM | yes | no | YMR only |

Table 2 : System tools are lacking in radionuclide transport and heat transport calculations in generic geologic media.

# Contributions from This Work

This work has provided a platform capable of bridging the gap between fuel cycle simulation and repository performance analysis.

- Conducted thermal transport sensitivity analyses. [14, 13]
- Conducted contaminant transport sensitivity analyses. [15]
- Cyder acheived integration with a fuel cycle simulator.
- Abstracted physical models of thermal and contaminant transport. [17]
- Demonstrated dominant physics of those models in Cyder, integrated with Cyclus. [18, 12]
- Published source code, documentation, and testing to facilitate extension by external developers. [16]

# Outline

# Cyder Paradigm : Waste Stream Acceptance

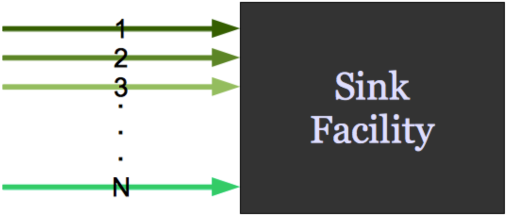


Figure 7 : To participate in a CYCLUS fuel cycle simulation, CYDER must accept **arbitrary** spent fuel and high level waste **material data objects**.

# Cyder Paradigm : Waste Stream Conditioning

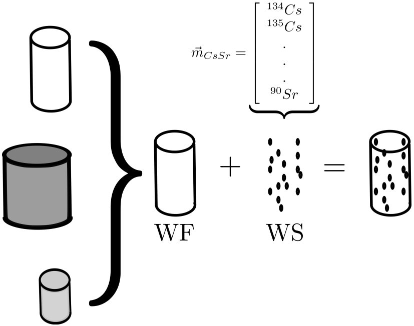


Figure 8 : In Cyder, discrete waste streams are conditioned into the appropriate discrete waste form according to user-specified pairings.

# Cyder Paradigm : Waste Form Packaging

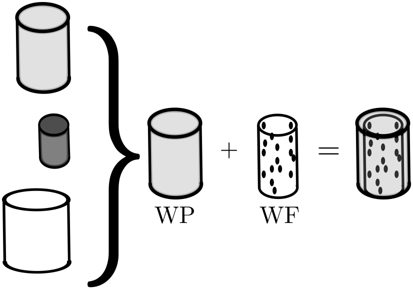


Figure 9 : In Cyder, one or more waste forms are loaded into the appropriate waste package according to user-specified pairings.

# Cyder Paradigm : Waste Package Emplacement

Finally, the waste package is **emplaced** in a buffer component, which contains many other waste packages, spaced evenly in a grid. The grid is defined by the user input and depends on repository depth, $\Delta z$, waste package spacing, $\Delta x$, and tunnel spacing, $\Delta y$ as in Figure 10.

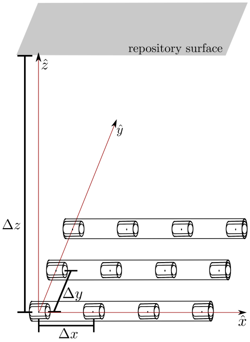
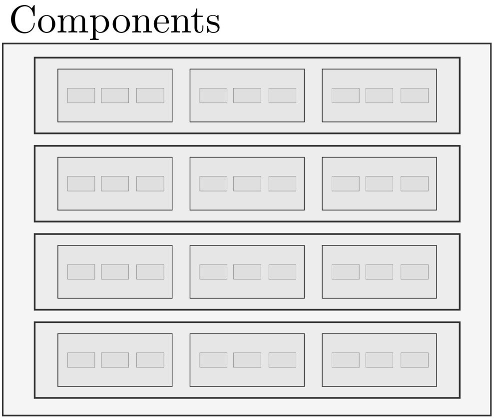
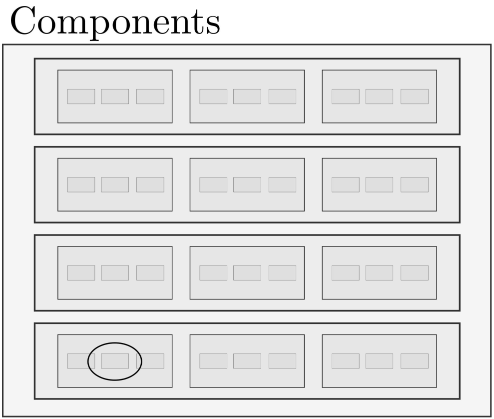


Figure 10 : The repository layout has a depth and a uniform package spacing.

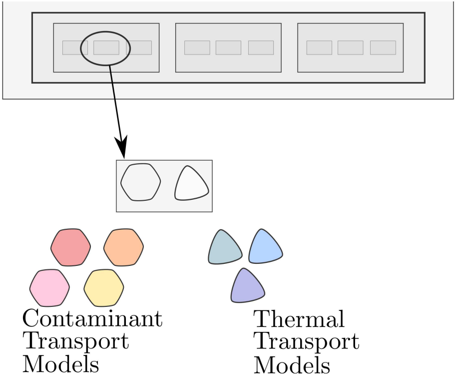
# Cyder Paradigm : Modularity



# Cyder Paradigm : Modularity



# Cyder Paradigm : Modularity



# Clay GDSM Sensitivity Analysis

- Barrier Degradation
- Sorption
- Solubility
- Advective Velocity
- Diffusivity

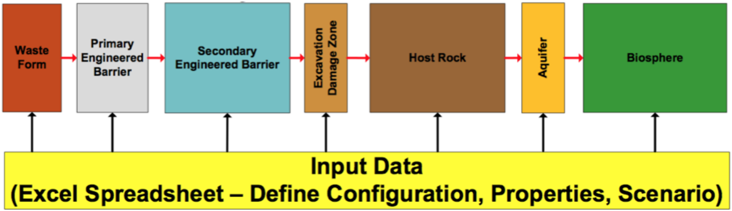


Figure 11 : The Clay Generic Disposal System Model (GDSM) was used for preliminary sensitivity analysis, abstraction iteration, and validation. This figure was reproduced from Figure 3.3-2 in [5].

# Nested Components

The NuclideModel in a Component can be interchangeably represented by any of the four nuclide transport models.

- Degradation Rate Based Failure Model
- Mixed Cell with Degradation, Sorption, Solubility Limitation
- Lumped Parameter Model
- 1 Dimensional Approximate Advection Dispersion Solution, Brenner [3]

# Radionuclide Transport: Degradation Rate Based Release

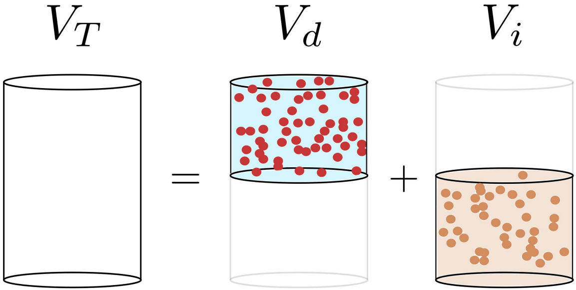


Figure 12 : The control volume contains an intact volume $V_i$ and a degraded volume, $V_d$. Contaminants in $V_d$ are available for transport, while contaminants in $V_i$ are contained.

# Radionuclide Transport : Mixed Cell with Sorption and Solubility

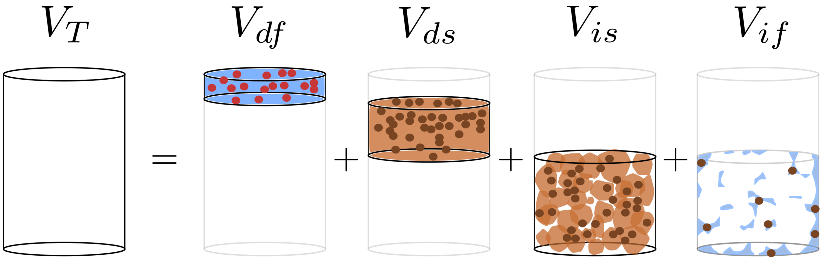


Figure 13 : The degraded volume is modeled as a solid degraded volume, $V_{ds}$, and a fluid degraded volume, $V_{df}$. The intact volume is modeled as an intact solid volume, $V_{is}$, and an intact fluid volume $V_{if}$. Only contaminants in $V_{df}$ are available for transport.

# Radionuclide Transport : Mixed Cell Sorption

The mass of contaminant sorbed into the degraded and precipitated solids can be found using a linear isotherm model [22], characterized by the relationship

$$s_i = K_{di} C_i \tag{1}$$

where

$$\begin{aligned} s_i = &\ \text{the solid concentration of isotope i } [kg/kg] \\ K_{di} = &\ \text{the distribution coefficient of isotope i}[m^3/kg] \\ C_i = &\ \text{the liquid concentration of isotope i } [kg/m^3]. \end{aligned}$$

# Radionuclide Transport : Mixed Cell Solubility Limitation

In addition to engineered barriers, contaminant transport is constrained by the solubility limit [11],

$$m_{s,i} \leq V_w C_{sol,i}, \tag{2}$$

where

$$\begin{aligned} m_{s,i} &= \text{ solubility limited mass of isotope i in volume } V_w[kg] \\ V_w &= \text{ volume of the solution } [m^3] \\ C_{sol,i} &= \text{ solubility limit, the maximum concentration of i } [kg/m^3]. \end{aligned}$$

# Radionuclide Transport: Lumped Parameter Transport Model

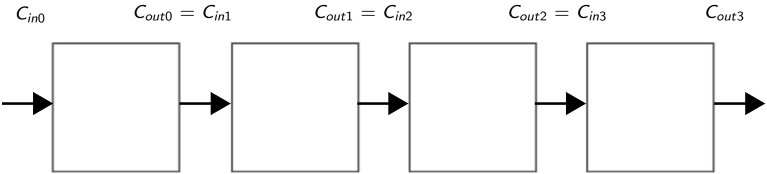


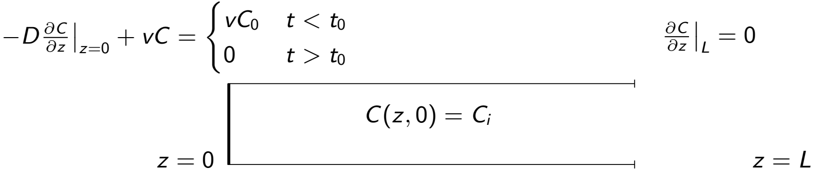
Figure 14 : The method by which each lumped parameter component is modeled is according to a relationship between the incoming concentration, $C_{in}(t)$, and the outgoing concentration, $C_{out}(t)$.

$$C_{out}(t) = \int_0^\infty C_{in}(t - t')g(t')e^{-\lambda t'} dt' \tag{3}$$

where

$$\begin{aligned} t' &= \text{time of entry } [s] \\ t - t' &= \text{transit time } [s] \\ g(t - t') &= \text{response function, a.k.a. transit time distribution}[-] \\ \lambda &= \text{radioactive decay constant}[s^{-1}]. \end{aligned}$$

# Radionuclide Transport: 1D Finite, Cauchy B.C.



$$-D\frac{\partial C}{\partial z}\Big|_{z=0} + vC = \begin{cases} vC_0 & t < t_0 \\ 0 & t > t_0 \end{cases}$$

$$\frac{\partial C}{\partial z}\Big|_{L} = 0$$

$$C(z,0) = C_i$$

$z = 0$

$z = L$

Figure 15 : A one dimensional, finite, unidirectional flow, solution with Cauchy and Neumann boundary conditions [25, 3].

# Clay GDSM Degradation Rate Sensitivity

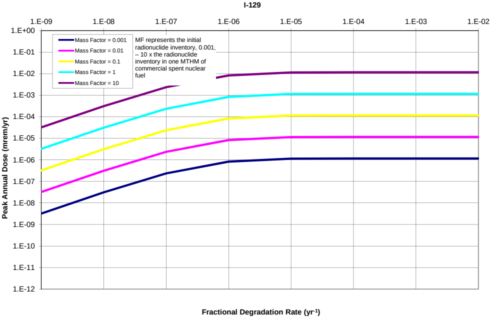


Figure 16 : $^{129}I$ waste form degradation rate sensitivity.

# Cyder Degradation Rate Sensitivity

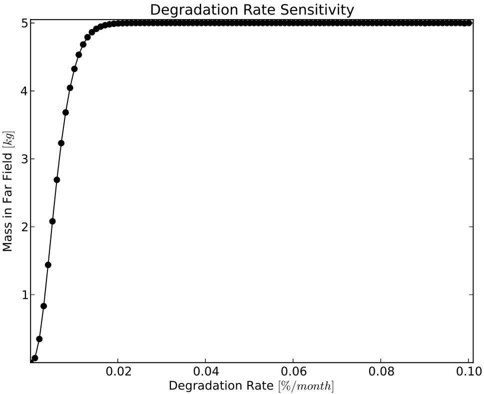


Figure 17 : Sensitivity demonstration of the degradation rate in CYDER for an arbitrary isotope.

# Clay GDSM Sorption Sensitivity

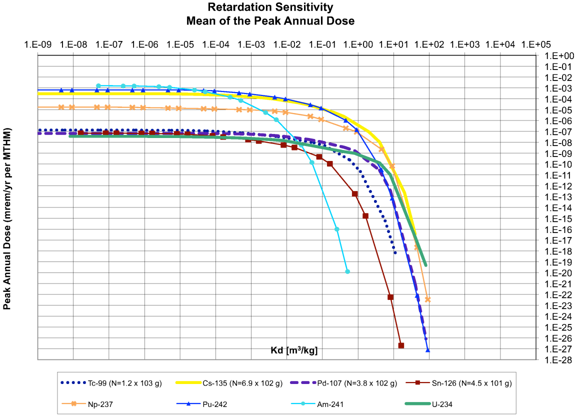


Figure 18 : $K_d$ sensitivity. The peak annual dose due to an inventory, $N$, of each isotope.

# Cyder Sorption Sensitivity

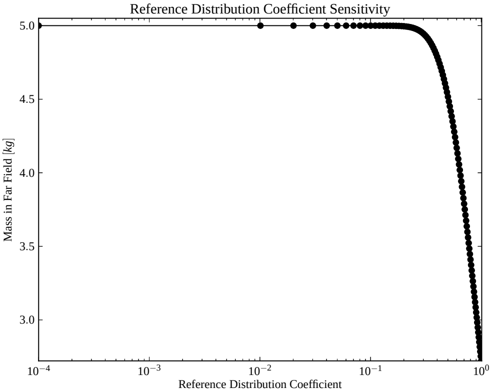


Figure 19 : $K_d$ factor sensitivity in the CYDER tool for an arbitrary isotope assigned a variable $K_d$ coefficient.

# Clay GDSM Solubility Sensitivity

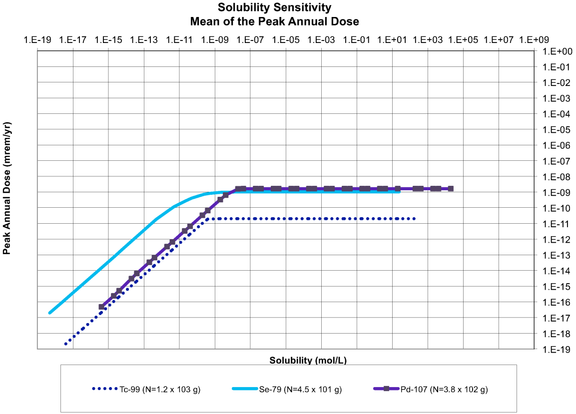


Figure 20 : Solubility limit sensitivity. The peak annual dose due to an inventory, *N*, of each isotope.

# Cyder Solubility Sensitivity

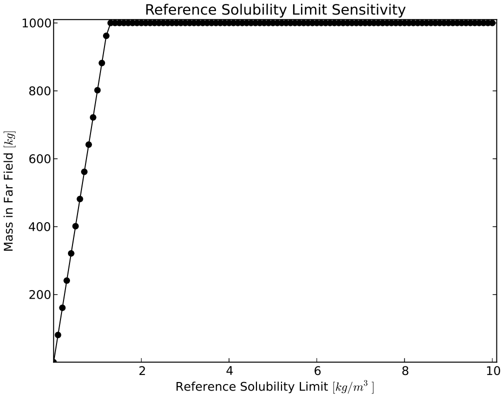


Figure 21 : Sensitivity demonstration of solubility limitation in CYDER for an arbitrary isotope assigned a variable solubility limit.

# Specific Temperature Change Calculations

A reference data set of temperature change curves was calculated. Repeated runs of a detailed model ([10, 8, 7]) over the range of values in Table 3 determined Specific Temperature Change (STC) values over that range.

**Thermal Cases**

| **Parameter** | **Symbol** | **Units** | **Value Range** |
|---|---|---|---|
| Diffusivity | $\alpha_{th}$ | $[m^2 \cdot s^{-1}]$ | $1.0 \times 10^{-7} - 3.0 \times 10^{-6}$ |
| Conductivity | $K_{th}$ | $[W \cdot m^{-1} \cdot K^{-1}]$ | $0.1 - 4.5$ |
| Spacing | $S$ | $[m]$ | 2, 5, 10, 15, 20, 25, 50 |
| Radius | $r_{lim}$ | $[m]$ | 0.1, 0.25, 0.5, 1, 2, 5 |
| Isotope | $i$ | $[-]$ | $^{241,243}Am$,<br>$^{242,243,244,245,246}Cm$,<br>$^{238,240,241,242}Pu$<br>$^{134,135,137}Cs$<br>$^{90}Sr$ |

Table 3 : A thermal reference dataset of STC values as a function of each of these parameters was generated by repeated parameterized runs of the LLNL MathCAD model[7, 8].

# Thermal Base Case Demonstration

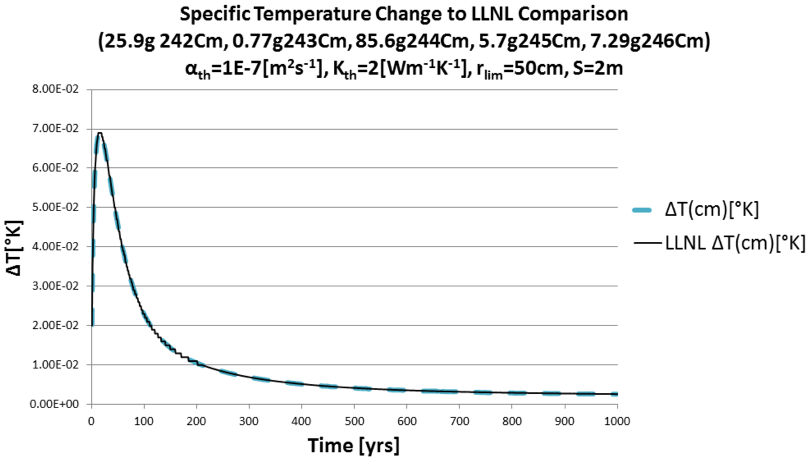


Figure 22 : This comparison of STC calculated thermal response from *Cm* inventory per MTHM in 51GWd burnup UOX PWR fuel compares favorably with results from the semi-analytic model from LLNL.

# Thermal Base Case Demonstration

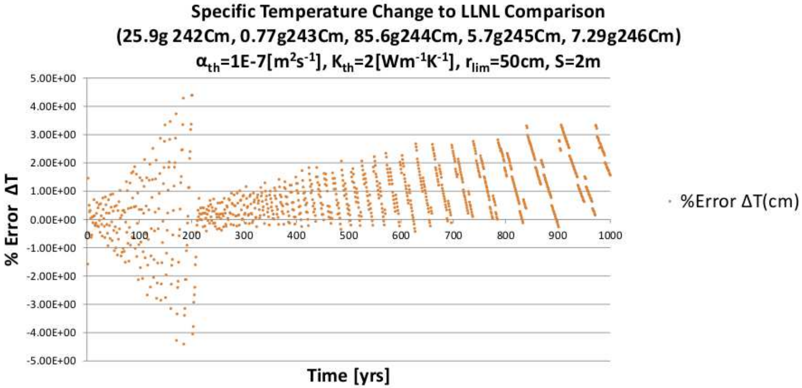


Figure 23 : Percent error between the semi-analytic model from LLNL and the STC calculated thermal response from *Cm* inventory per MTHM in 51GWd burnup UOX PWR fuel demonstrates a maximum percent error of 4.4%.

# LLNL Model Thermal Conductivity Sensitivity

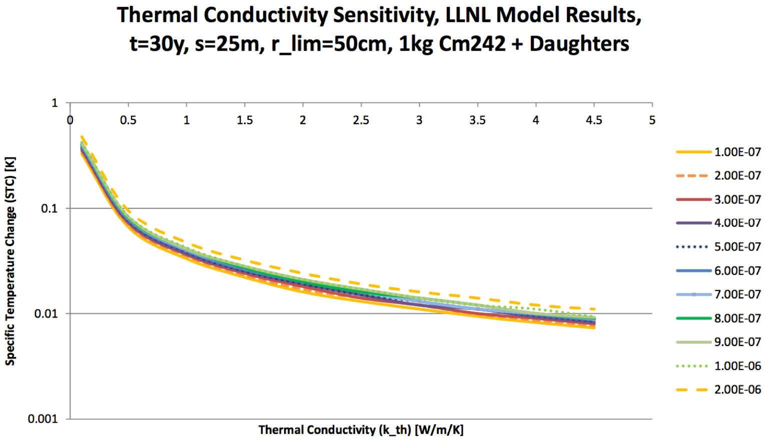


Figure 24 : Increased thermal conductivity decreases the temperature (here represented by STC) at the limiting radius.

# Cyder Thermal Conductivity Sensitivity

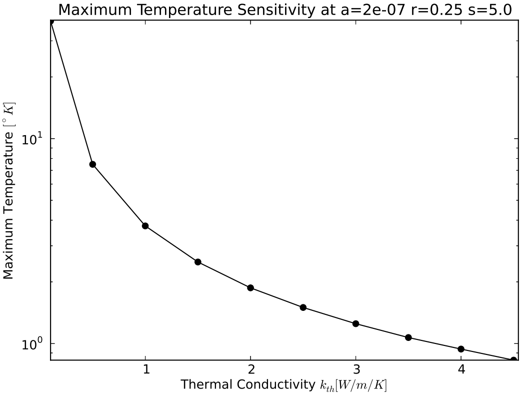


Figure 25 : Cyder results agree with those of the LLNL model. Increased $K_{th}$ decreases temperature change at the limiting radius. The above example thermal profile results from 10kg of $^{242}Cm$, $\alpha_{th} = 2 \times 10^{-7}$, $s = 5m$, and $r_{lim} = 0.25m$.

# LLNL Model Thermal Diffusivity Sensitivity

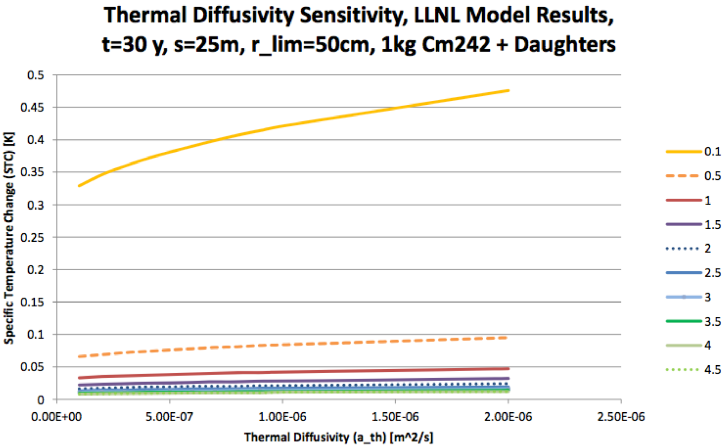


Figure 26 : Increased thermal diffusivity decreases temperature change (here represented by STC) at the limiting radius (here $r_{calc} = 0.5m$).

# Cyder Thermal Diffusivity Sensitivity

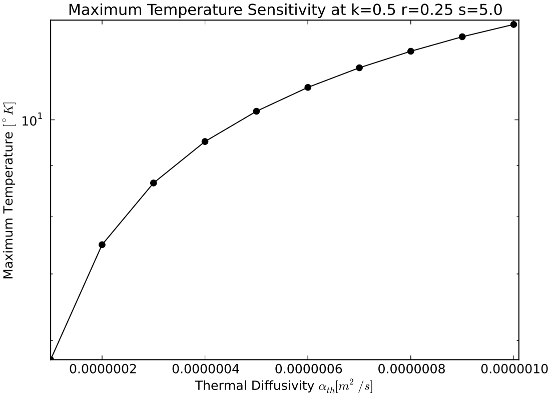


Figure 27 : Cyder trends agree with those of the LLNL model, in which increased thermal diffusivity results in reduced temperature change at the limiting radius. The above example thermal profile results from 10kg of $^{242}Cm$.

# Outline

# Conclusion : Summary of Contributions

This work has provided a software platform capable of bridging the gap between fuel cycle simulation and repository performance analysis.

- Conducted thermal transport sensitivity analyses. [14, 13]
- Conducted contaminant transport sensitivity analyses. [15]
- Cyder acheived integration with a fuel cycle simulator.
- Abstracted physical models of thermal and contaminant transport. [17]
- Demonstrated dominant physics of those models in Cyder, integrated with Cyclus. [18, 12]
- Published source code, documentation, and testing to facilitate extension by external developers. [16]

# Conclusion : Suggested Future Work

Further work could include

- cultivation of a developer community,
- more detailed benchmarking validation against sophisticated tools,
- comparison against experimental data, where available,
- demonstration of dynamic fuel cycle feedback sensitivities,
- additional physics (fracture models, biosphere models),
- and additional supporting data.

# Acknowledgements

This work was carried out with the generous support of the **UFD Campaign** at **Argonne National Laboratory.** This work is supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Nuclear Energy, under contract # DE-AC02-06CH11357.

Figure 28 : This work relied on Cyclus, the next generation fuel cycle simulator, and its team. `cyclus.github.com`

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